



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:50 AM UTC

PDB ID : 6OYH / pdb_00006oyh
Title : Crystal structure of MraY bound to carbacaprazamycin
Authors : Mashalidis, E.H.; Lee, S.Y.
Deposited on : 2019-05-14
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

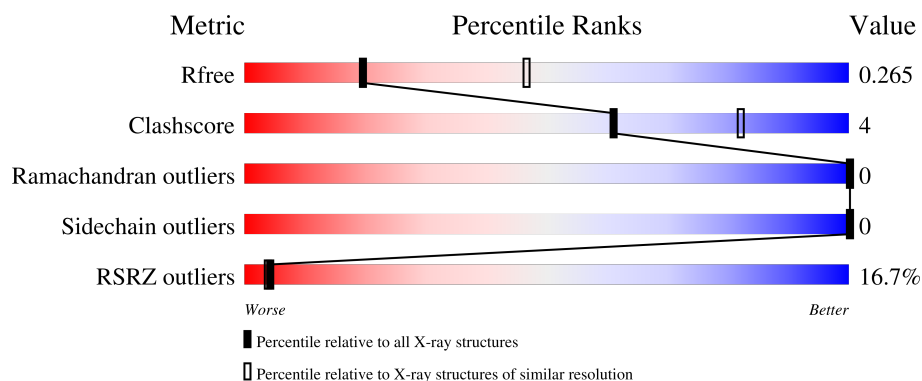
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	137	
1	F	137	
1	G	137	
1	H	137	
2	A	365	

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Mol	Chain	Length	Quality of chain
2	B	365	15% 84% 7% 10%
2	C	365	16% 79% 11% 10%
2	D	365	19% 82% 10% 8%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 27565 atoms, of which 13714 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MraYAA nanobody.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	124	Total	C	H	N	O	S	0	0	0
			1800	580	872	160	184	4			
1	G	125	Total	C	H	N	O	S	0	0	0
			1760	573	847	157	179	4			
1	F	125	Total	C	H	N	O	S	0	0	0
			1812	584	878	160	186	4			
1	H	126	Total	C	H	N	O	S	0	0	0
			1794	580	864	162	184	4			

- Molecule 2 is a protein called Phospho-N-acetylmuramoyl-pentapeptide-transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	326	Total	C	H	N	O	S	0	0	0
			5046	1682	2558	379	419	8			
2	C	328	Total	C	H	N	O	S	0	0	0
			4949	1656	2487	379	419	8			
2	B	330	Total	C	H	N	O	S	0	0	0
			4998	1678	2511	380	422	7			
2	D	337	Total	C	H	N	O	S	0	0	0
			4902	1656	2433	379	426	8			

There are 24 discrepancies between the modelled and reference sequences:

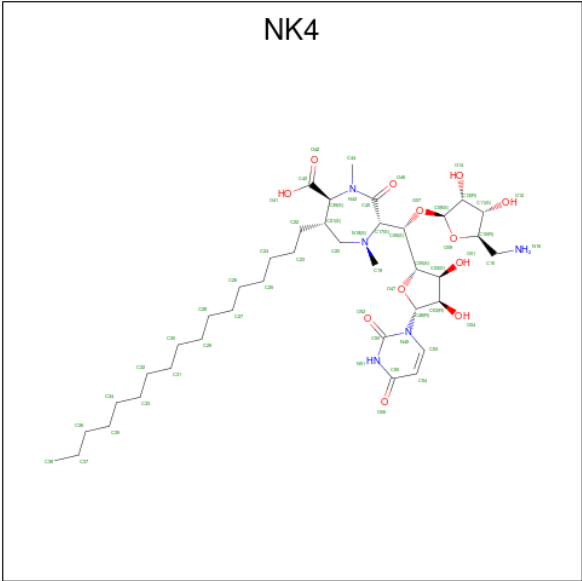
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP O66465
A	-4	PRO	-	expression tag	UNP O66465
A	-3	ALA	-	expression tag	UNP O66465
A	-2	VAL	-	expression tag	UNP O66465
A	-1	PRO	-	expression tag	UNP O66465
A	0	ARG	-	expression tag	UNP O66465
C	-5	GLY	-	expression tag	UNP O66465
C	-4	PRO	-	expression tag	UNP O66465

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	ALA	-	expression tag	UNP O66465
C	-2	VAL	-	expression tag	UNP O66465
C	-1	PRO	-	expression tag	UNP O66465
C	0	ARG	-	expression tag	UNP O66465
B	-5	GLY	-	expression tag	UNP O66465
B	-4	PRO	-	expression tag	UNP O66465
B	-3	ALA	-	expression tag	UNP O66465
B	-2	VAL	-	expression tag	UNP O66465
B	-1	PRO	-	expression tag	UNP O66465
B	0	ARG	-	expression tag	UNP O66465
D	-5	GLY	-	expression tag	UNP O66465
D	-4	PRO	-	expression tag	UNP O66465
D	-3	ALA	-	expression tag	UNP O66465
D	-2	VAL	-	expression tag	UNP O66465
D	-1	PRO	-	expression tag	UNP O66465
D	0	ARG	-	expression tag	UNP O66465

- Molecule 3 is (5S)-5'-O-(5-amino-5-deoxy-beta-D-ribofuranosyl)-5'-C-[(2S,5S,6S)-5-carboxy-6-heptadecyl-1,4-dimethyl-3-oxo-1,4-diazepan-2-yl]uridine (CCD ID: NK4) (formula: C₃₉H₆₇N₅O₁₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			122	39	66	5	12		
3	C	1	Total	C	H	N	O	0	0
			122	39	66	5	12		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	H	N	O	0	0
			122	39	66	5	12		
3	D	1	Total	C	H	N	O	0	0
			122	39	66	5	12		

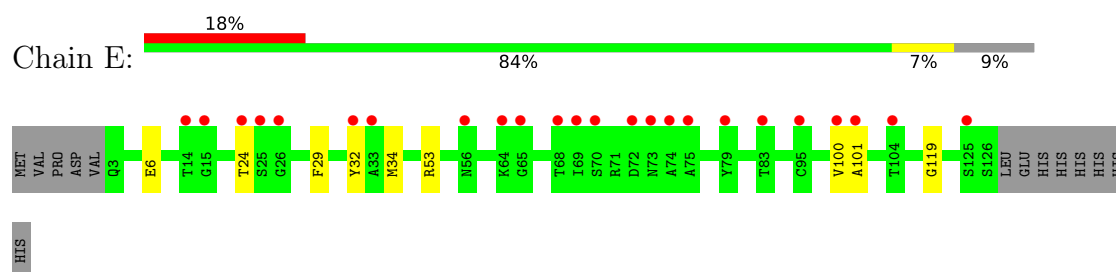
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	2	Total	O	0	0
			2	2		
4	A	5	Total	O	0	0
			5	5		
4	C	6	Total	O	0	0
			6	6		
4	B	1	Total	O	0	0
			1	1		
4	D	2	Total	O	0	0
			2	2		

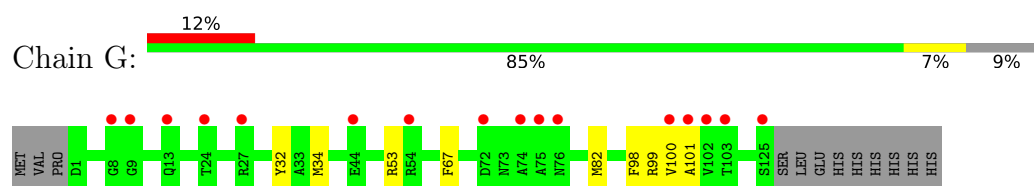
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

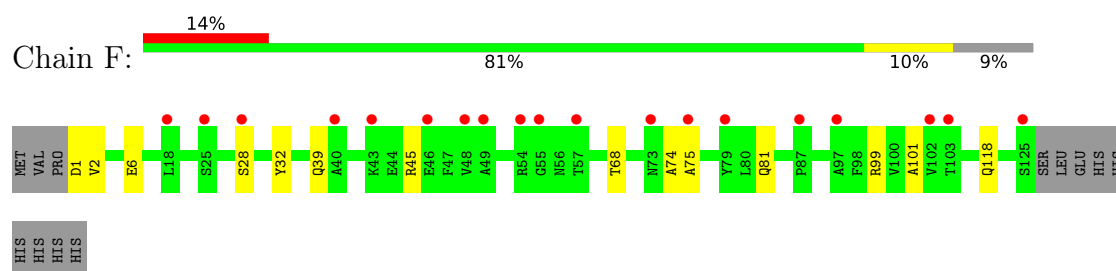
- Molecule 1: MraYAA nanobody



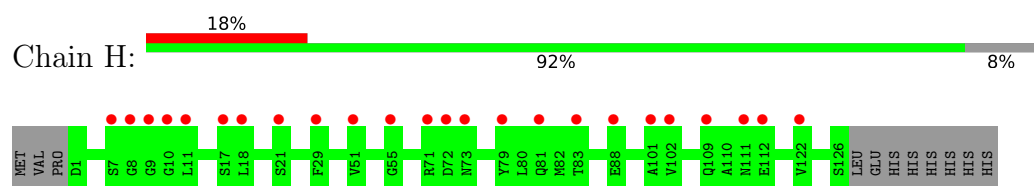
- Molecule 1: MraYAA nanobody



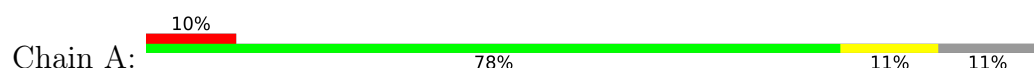
- Molecule 1: MraYAA nanobody

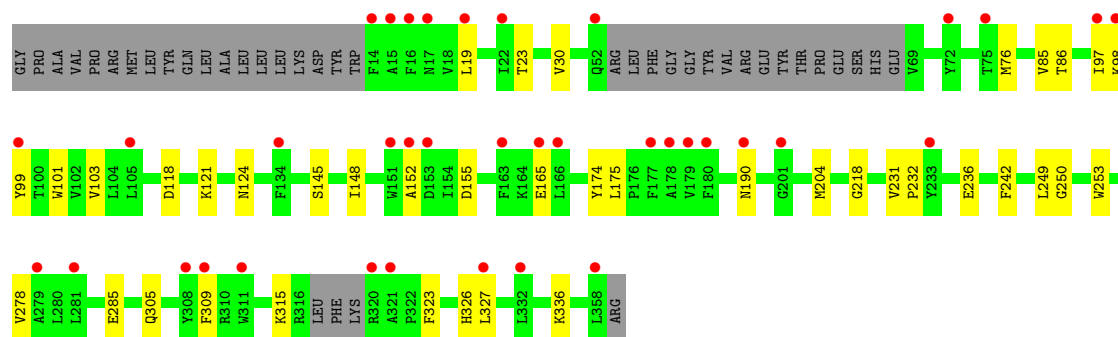


- Molecule 1: MraYAA nanobody

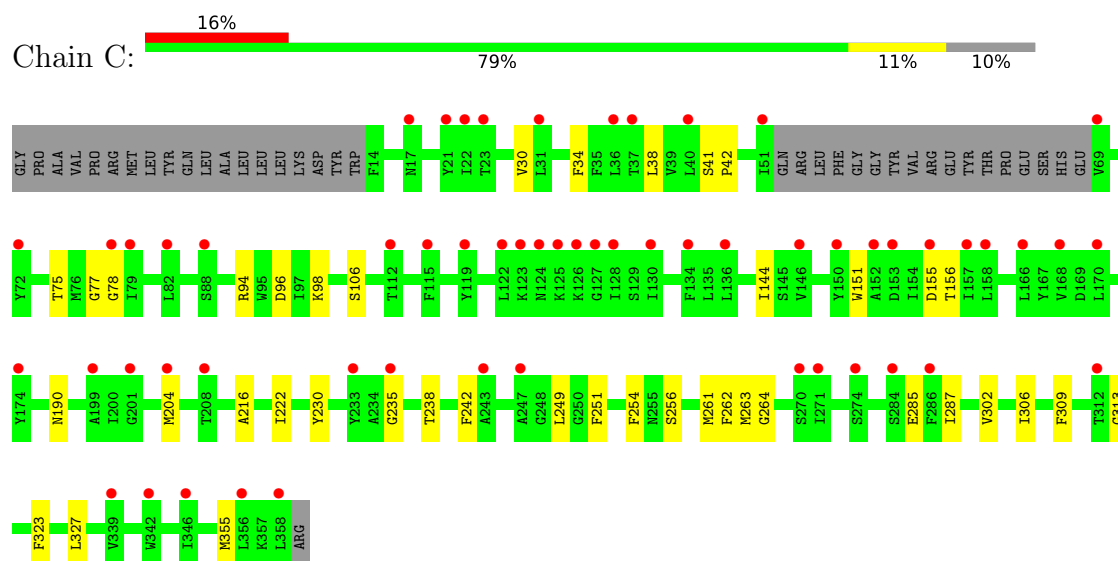


- Molecule 2: Phospho-N-acetylmuramoyl-pentapeptide-transferase

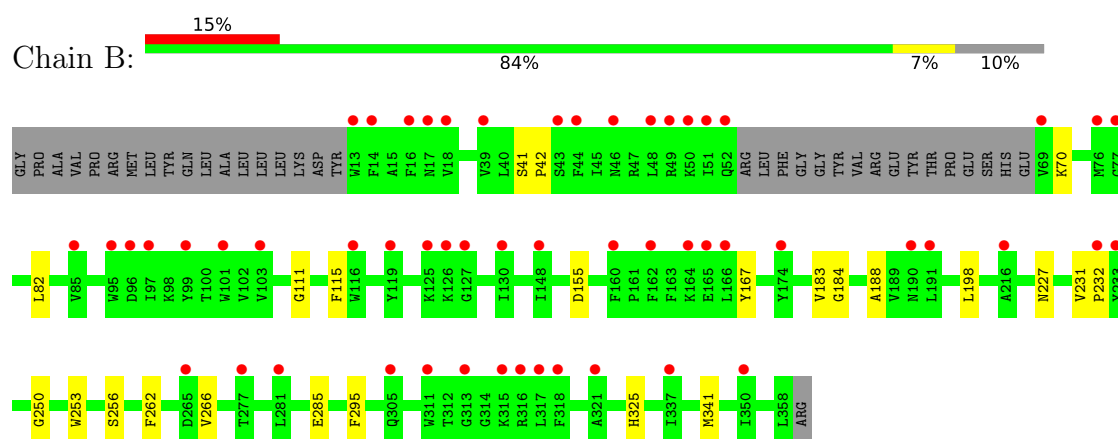




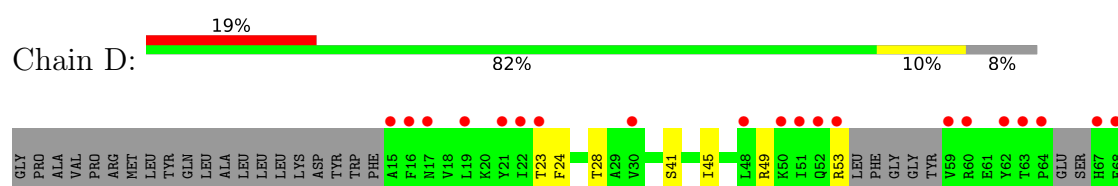
• Molecule 2: Phospho-N-acetylmuramoyl-pentapeptide-transferase

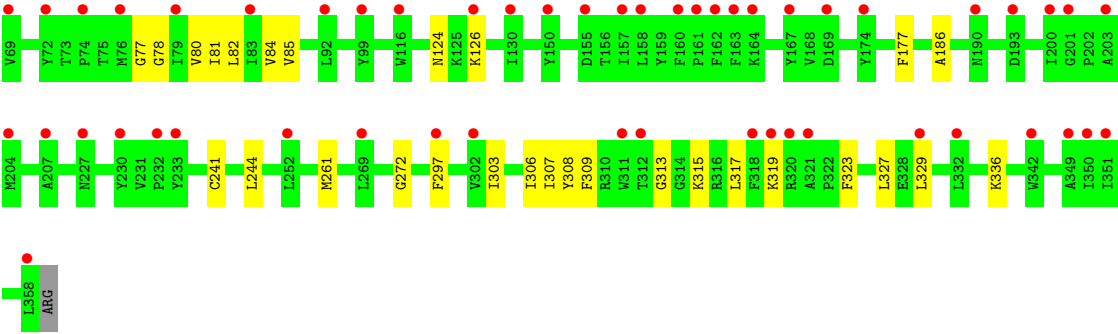


• Molecule 2: Phospho-N-acetylmuramoyl-pentapeptide-transferase



• Molecule 2: Phospho-N-acetylmuramoyl-pentapeptide-transferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.89Å 129.58Å 129.43Å 90.00° 109.33° 90.00°	Depositor
Resolution (Å)	43.94 – 2.95 43.94 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (43.94-2.95) 90.2 (43.94-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.93 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.248 , 0.268 (Not available) , 0.265	Depositor DCC
R_{free} test set	2632 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	27565	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NK4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	E	0.19	0/946	0.35	0/1285
1	F	0.20	0/952	0.41	0/1294
1	G	0.21	0/931	0.39	0/1267
1	H	0.23	0/948	0.38	0/1291
2	A	0.26	0/2550	0.50	0/3480
2	B	0.16	0/2550	0.35	0/3492
2	C	0.41	1/2522 (0.0%)	0.57	1/3447 (0.0%)
2	D	0.34	0/2527	0.60	0/3463
All	All	0.28	1/13926 (0.0%)	0.48	1/19019 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	156	THR	C-O	-5.10	1.16	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	156	THR	N-CA-C	-5.01	104.10	111.81

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	928	872	872	5	0
1	F	934	878	880	11	0
1	G	913	847	849	10	0
1	H	930	864	866	0	0
2	A	2488	2558	2559	26	0
2	B	2487	2511	2511	16	0
2	C	2462	2487	2486	29	0
2	D	2469	2433	2435	27	0
3	A	56	66	0	1	0
3	B	56	66	0	1	0
3	C	56	66	0	3	0
3	D	56	66	0	0	0
4	A	5	0	0	0	0
4	B	1	0	0	0	0
4	C	6	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
All	All	13851	13714	13458	114	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (114) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:308:TYR:CD1	2:D:317:LEU:HD21	2.14	0.82
2:B:285:GLU:N	2:B:285:GLU:OE1	2.24	0.70
2:A:305:GLN:OE1	2:A:315:LYS:CB	2.41	0.69
2:C:256:SER:O	2:D:336:LYS:NZ	2.25	0.68
2:A:165:GLU:N	2:A:165:GLU:OE1	2.31	0.63
2:D:308:TYR:CG	2:D:317:LEU:HG	2.34	0.63
2:A:19:LEU:O	2:A:23:THR:HG22	1.98	0.63
2:A:305:GLN:CD	2:A:315:LYS:CB	2.72	0.62
2:D:309:PHE:O	2:D:313:GLY:O	2.19	0.61
2:C:251:PHE:CZ	2:C:263:MET:HB2	2.37	0.60
1:E:101:ALA:O	2:A:155:ASP:N	2.35	0.60
2:A:190:ASN:OD1	3:A:401:NK4:N16	2.36	0.58
2:D:309:PHE:HA	2:D:315:LYS:O	2.03	0.58
2:C:264:GLY:N	3:C:401:NK4:O12	2.37	0.57
2:A:174:TYR:OH	2:A:285:GLU:OE2	2.24	0.56
2:A:145:SER:HB3	2:A:175:LEU:HD23	1.89	0.55
2:A:305:GLN:HA	2:A:315:LYS:CB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:308:TYR:CD1	2:D:317:LEU:CD2	2.89	0.55
2:C:285:GLU:OE1	2:C:285:GLU:N	2.31	0.54
2:C:77:GLY:HA3	2:C:261:MET:HE2	1.90	0.52
1:F:99:ARG:NH2	2:B:227:ASN:OD1	2.42	0.52
2:D:241:CYS:O	2:D:244:LEU:HB3	2.10	0.52
2:C:75:THR:OG1	3:C:401:NK4:O14	2.21	0.52
2:C:98:LYS:HB2	2:C:151:TRP:CH2	2.46	0.50
1:F:39:GLN:OE1	1:F:45:ARG:HG3	2.12	0.50
2:B:188:ALA:HB1	2:B:295:PHE:HB3	1.94	0.49
2:D:78:GLY:O	2:D:82:LEU:HD13	2.13	0.49
2:D:303:ILE:O	2:D:306:ILE:HG22	2.12	0.49
1:G:32:TYR:CE1	1:G:99:ARG:HG3	2.48	0.48
2:C:41:SER:HB2	2:C:254:PHE:CE2	2.48	0.48
2:D:308:TYR:CD2	2:D:317:LEU:HG	2.47	0.48
1:G:32:TYR:CD1	1:G:99:ARG:HG3	2.48	0.48
1:F:28:SER:HB3	2:B:167:TYR:OH	2.12	0.48
1:E:53:ARG:NH1	1:E:100:VAL:O	2.45	0.48
2:D:49:ARG:O	2:D:53:ARG:O	2.32	0.48
1:G:32:TYR:HB2	1:G:34:MET:HE3	1.96	0.48
2:A:98:LYS:HA	2:A:101:TRP:HD1	1.79	0.48
1:F:101:ALA:O	2:B:155:ASP:HB2	2.13	0.48
2:B:115:PHE:CA	2:B:266:VAL:HG22	2.44	0.47
1:E:6:GLU:OE1	1:E:119:GLY:N	2.47	0.47
2:C:34:PHE:CE2	2:C:38:LEU:HD11	2.49	0.47
2:C:204:MET:HE1	2:C:249:LEU:HD23	1.96	0.47
2:C:34:PHE:CZ	2:C:38:LEU:HD11	2.49	0.47
2:A:323:PHE:CE1	2:A:326:HIS:HD2	2.32	0.47
2:D:297:PHE:HE2	2:D:323:PHE:CG	2.33	0.47
2:D:23:THR:HG1	2:D:28:THR:HG1	1.60	0.47
2:B:70:LYS:HG2	2:B:262:PHE:HZ	1.80	0.47
1:G:101:ALA:O	2:C:155:ASP:N	2.46	0.46
2:C:94:ARG:NH1	2:C:96:ASP:OD2	2.48	0.46
1:G:67:PHE:CE1	1:G:82:MET:HB2	2.50	0.46
2:D:41:SER:O	2:D:45:ILE:HG12	2.16	0.46
2:D:306:ILE:HG23	2:D:307:ILE:N	2.31	0.46
2:D:124:ASN:ND2	2:D:126:LYS:O	2.47	0.46
2:C:235:GLY:O	2:C:238:THR:HB	2.15	0.46
2:D:77:GLY:HA3	2:D:261:MET:HE2	1.98	0.45
2:B:115:PHE:N	2:B:266:VAL:HG22	2.31	0.45
2:A:323:PHE:CZ	2:A:327:LEU:HD11	2.50	0.45
1:G:101:ALA:O	2:C:155:ASP:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:309:PHE:O	2:C:313:GLY:O	2.34	0.45
2:B:250:GLY:O	2:B:253:TRP:HB3	2.17	0.45
2:C:323:PHE:CE2	2:C:327:LEU:CD1	3.00	0.45
1:G:53:ARG:NH1	1:G:100:VAL:O	2.48	0.45
2:A:19:LEU:HD23	2:A:19:LEU:HA	1.89	0.44
2:C:323:PHE:CE2	2:C:327:LEU:HD11	2.52	0.44
2:B:325:HIS:NE2	3:B:401:NK4:O42	2.45	0.44
2:C:106:SER:HA	2:C:144:ILE:HD11	2.00	0.44
2:A:85:VAL:O	2:A:86:THR:C	2.61	0.44
2:A:97:ILE:HG13	2:A:236:GLU:HG3	2.00	0.44
2:D:308:TYR:CE1	2:D:317:LEU:HD21	2.51	0.44
2:C:78:GLY:N	2:C:263:MET:O	2.35	0.43
2:D:23:THR:OG1	2:D:28:THR:OG1	2.29	0.43
2:D:297:PHE:HE2	2:D:323:PHE:CD2	2.37	0.43
2:C:190:ASN:OD1	3:C:401:NK4:N16	2.52	0.43
1:F:1:ASP:OD1	1:F:2:VAL:N	2.51	0.43
2:B:82:LEU:HD21	2:B:111:GLY:HA3	2.00	0.43
2:C:302:VAL:O	2:C:306:ILE:HG22	2.18	0.43
2:A:148:ILE:O	2:A:152:ALA:O	2.36	0.43
2:C:287:ILE:HA	2:C:355:MET:CE	2.49	0.43
2:D:24:PHE:O	2:D:28:THR:OG1	2.37	0.43
1:F:32:TYR:CE2	1:F:99:ARG:HG3	2.54	0.42
2:D:323:PHE:CE2	2:D:327:LEU:HD11	2.53	0.42
2:A:309:PHE:CD2	2:A:309:PHE:C	2.97	0.42
2:A:76:MET:SD	2:A:118:ASP:HB3	2.58	0.42
2:C:75:THR:HA	2:C:262:PHE:HB2	2.01	0.42
1:F:74:ALA:O	1:F:75:ALA:HB3	2.18	0.42
1:F:28:SER:O	1:F:28:SER:OG	2.36	0.42
2:A:99:TYR:HE2	2:A:232:PRO:O	2.01	0.42
2:D:186:ALA:HA	2:D:272:GLY:HA3	2.00	0.42
1:E:24:THR:HG21	1:E:32:TYR:HE1	1.85	0.41
2:A:30:VAL:HG23	2:A:242:PHE:HB3	2.02	0.41
2:A:250:GLY:O	2:A:253:TRP:HB3	2.21	0.41
1:E:29:PHE:CE1	1:E:34:MET:HE2	2.55	0.41
2:A:121:LYS:HA	2:A:124:ASN:O	2.20	0.41
1:G:100:VAL:HG12	2:C:230:TYR:CD2	2.54	0.41
1:G:100:VAL:HG12	2:C:230:TYR:HD2	1.85	0.41
2:B:183:VAL:O	2:B:184:GLY:C	2.62	0.41
2:D:177:PHE:CD2	2:D:177:PHE:C	2.98	0.41
2:C:216:ALA:HA	2:C:222:ILE:HG21	2.02	0.41
1:F:118:GLN:OE1	1:F:118:GLN:N	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:231:VAL:O	2:B:232:PRO:C	2.64	0.41
2:C:30:VAL:HG23	2:C:242:PHE:HB3	2.01	0.41
2:D:84:VAL:O	2:D:85:VAL:C	2.64	0.41
2:A:103:VAL:HG21	2:A:278:VAL:HG23	2.03	0.41
2:A:218:GLY:HA2	2:A:231:VAL:O	2.20	0.41
1:G:98:PHE:CE1	1:G:100:VAL:CG1	3.04	0.41
1:F:6:GLU:OE1	1:F:6:GLU:N	2.53	0.41
1:F:68:THR:OG1	1:F:81:GLN:HG2	2.21	0.41
2:B:41:SER:N	2:B:42:PRO:CD	2.84	0.41
2:A:336:LYS:NZ	2:B:256:SER:O	2.53	0.41
2:C:38:LEU:O	2:C:42:PRO:HD3	2.21	0.40
2:B:198:LEU:HD11	2:B:341:MET:HG3	2.03	0.40
2:D:319:LYS:CB	2:D:329:LEU:HD12	2.52	0.40
2:D:80:VAL:O	2:D:81:ILE:C	2.64	0.40
2:A:204:MET:HE1	2:A:249:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	122/137 (89%)	122 (100%)	0	0	100	100
1	F	123/137 (90%)	119 (97%)	4 (3%)	0	100	100
1	G	123/137 (90%)	119 (97%)	4 (3%)	0	100	100
1	H	124/137 (90%)	123 (99%)	1 (1%)	0	100	100
2	A	320/365 (88%)	301 (94%)	19 (6%)	0	100	100
2	B	326/365 (89%)	307 (94%)	19 (6%)	0	100	100
2	C	324/365 (89%)	311 (96%)	13 (4%)	0	100	100
2	D	331/365 (91%)	315 (95%)	16 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1793/2008 (89%)	1717 (96%)	76 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	93/110 (84%)	93 (100%)	0	100	100
1	F	94/110 (86%)	94 (100%)	0	100	100
1	G	88/110 (80%)	88 (100%)	0	100	100
1	H	92/110 (84%)	92 (100%)	0	100	100
2	A	259/309 (84%)	259 (100%)	0	100	100
2	B	253/309 (82%)	253 (100%)	0	100	100
2	C	250/309 (81%)	250 (100%)	0	100	100
2	D	243/309 (79%)	243 (100%)	0	100	100
All	All	1372/1676 (82%)	1372 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	13	GLN
2	A	137	GLN
2	A	326	HIS
2	D	324	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NK4	A	401	-	52,59,59	3.79	8 (15%)	57,81,81	1.87	14 (24%)
3	NK4	C	401	-	52,59,59	3.86	8 (15%)	57,81,81	1.76	9 (15%)
3	NK4	D	401	-	52,59,59	3.91	8 (15%)	57,81,81	1.65	10 (17%)
3	NK4	B	401	-	52,59,59	3.86	8 (15%)	57,81,81	1.93	14 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NK4	A	401	-	-	12/33/95/95	0/3/4/4
3	NK4	C	401	-	-	10/33/95/95	0/3/4/4
3	NK4	D	401	-	-	13/33/95/95	0/3/4/4
3	NK4	B	401	-	-	9/33/95/95	0/3/4/4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	NK4	C45-N43	-23.10	1.11	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	NK4	C45-N43	-23.02	1.11	1.35
3	B	401	NK4	C45-N43	-23.02	1.11	1.35
3	A	401	NK4	C45-N43	-22.24	1.12	1.35
3	D	401	NK4	C50-N49	-7.78	1.26	1.38
3	D	401	NK4	C55-N51	-7.78	1.25	1.38
3	B	401	NK4	C50-N49	-7.68	1.26	1.38
3	C	401	NK4	C50-N49	-7.64	1.26	1.38
3	A	401	NK4	C50-N49	-7.62	1.26	1.38
3	A	401	NK4	C55-N51	-7.54	1.25	1.38
3	C	401	NK4	C55-N51	-7.24	1.26	1.38
3	B	401	NK4	C55-N51	-7.23	1.26	1.38
3	A	401	NK4	C50-N51	-6.81	1.26	1.38
3	D	401	NK4	C50-N51	-6.79	1.26	1.38
3	B	401	NK4	C50-N51	-6.72	1.26	1.38
3	C	401	NK4	C50-N51	-6.59	1.26	1.38
3	A	401	NK4	C53-N49	-5.35	1.25	1.38
3	B	401	NK4	C53-N49	-5.31	1.25	1.38
3	D	401	NK4	C53-N49	-5.22	1.25	1.38
3	C	401	NK4	C53-N49	-5.20	1.25	1.38
3	D	401	NK4	C54-C55	-4.66	1.33	1.43
3	B	401	NK4	C54-C55	-4.58	1.33	1.43
3	A	401	NK4	C54-C55	-4.49	1.33	1.43
3	C	401	NK4	C54-C55	-4.41	1.34	1.43
3	C	401	NK4	C08-C13	-4.00	1.47	1.52
3	D	401	NK4	C08-C13	-3.99	1.47	1.52
3	A	401	NK4	C08-C13	-3.84	1.48	1.52
3	B	401	NK4	C08-C13	-3.41	1.48	1.52
3	A	401	NK4	C17-N18	2.25	1.48	1.47
3	D	401	NK4	C17-N18	2.14	1.48	1.47
3	C	401	NK4	C17-N18	2.01	1.48	1.47
3	B	401	NK4	C17-N18	2.01	1.48	1.47

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NK4	N51-C50-N49	5.69	122.30	114.89
3	C	401	NK4	N51-C50-N49	5.49	122.03	114.89
3	D	401	NK4	N51-C50-N49	5.43	121.97	114.89
3	B	401	NK4	N51-C50-N49	5.33	121.83	114.89
3	B	401	NK4	O41-C40-C39	5.00	120.20	111.92
3	A	401	NK4	O41-C40-C39	4.69	119.68	111.92
3	A	401	NK4	C55-N51-C50	-4.66	120.83	126.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	NK4	O41-C40-C39	4.59	119.52	111.92
3	B	401	NK4	C55-N51-C50	-4.59	120.92	126.61
3	C	401	NK4	C55-N51-C50	-4.59	120.92	126.61
3	C	401	NK4	O41-C40-C39	4.54	119.43	111.92
3	A	401	NK4	O46-C45-N43	-4.31	116.83	121.68
3	D	401	NK4	C55-N51-C50	-4.02	121.63	126.61
3	B	401	NK4	O46-C45-N43	-3.62	117.60	121.68
3	B	401	NK4	O56-C55-C54	-3.55	119.03	125.16
3	D	401	NK4	O46-C45-N43	-3.55	117.68	121.68
3	B	401	NK4	C02-C05-C06	-3.34	111.07	115.75
3	A	401	NK4	C02-C05-C06	-3.27	111.17	115.75
3	C	401	NK4	O46-C45-N43	-3.25	118.02	121.68
3	B	401	NK4	C54-C55-N51	3.22	119.31	114.80
3	C	401	NK4	O56-C55-C54	-3.13	119.77	125.16
3	A	401	NK4	C54-C55-N51	3.06	119.09	114.80
3	C	401	NK4	C02-C05-C06	-3.01	111.53	115.75
3	B	401	NK4	C08-C13-C11	2.99	106.01	102.29
3	C	401	NK4	C54-C55-N51	2.98	118.97	114.80
3	C	401	NK4	O52-C50-N49	-2.86	119.07	122.80
3	A	401	NK4	O56-C55-C54	-2.83	120.28	125.16
3	A	401	NK4	O42-C40-C39	-2.82	119.37	123.45
3	C	401	NK4	C15-C10-C11	-2.80	108.28	114.95
3	B	401	NK4	O09-C08-C13	2.79	108.53	104.98
3	D	401	NK4	C54-C55-N51	2.71	118.60	114.80
3	B	401	NK4	O47-C05-C02	2.54	108.94	104.21
3	D	401	NK4	C02-C05-C06	-2.53	112.21	115.75
3	D	401	NK4	O56-C55-C54	-2.52	120.81	125.16
3	B	401	NK4	O42-C40-C39	-2.52	119.81	123.45
3	B	401	NK4	O52-C50-N49	-2.52	119.52	122.80
3	A	401	NK4	O52-C50-N49	-2.46	119.59	122.80
3	D	401	NK4	O52-C50-N49	-2.46	119.60	122.80
3	A	401	NK4	C15-C10-C11	-2.44	109.15	114.95
3	B	401	NK4	C15-C10-C11	-2.31	109.45	114.95
3	B	401	NK4	C48-N49-C50	2.24	121.62	117.59
3	A	401	NK4	C48-N49-C50	2.23	121.59	117.59
3	A	401	NK4	O09-C08-C13	2.21	107.79	104.98
3	D	401	NK4	C15-C10-C11	-2.19	109.74	114.95
3	A	401	NK4	C02-C03-C48	2.17	105.56	101.46
3	D	401	NK4	O42-C40-C39	-2.14	120.36	123.45
3	A	401	NK4	C08-C13-C11	2.03	104.82	102.29

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	NK4	C20-C21-C22-C23
3	A	401	NK4	C13-C08-O07-C06
3	C	401	NK4	C20-C21-C22-C23
3	C	401	NK4	C13-C08-O07-C06
3	B	401	NK4	C20-C21-C22-C23
3	D	401	NK4	C20-C21-C22-C23
3	D	401	NK4	C13-C08-O07-C06
3	D	401	NK4	C32-C33-C34-C35
3	A	401	NK4	C32-C33-C34-C35
3	C	401	NK4	C32-C33-C34-C35
3	B	401	NK4	C32-C33-C34-C35
3	B	401	NK4	C21-C22-C23-C24
3	D	401	NK4	C24-C25-C26-C27
3	C	401	NK4	C24-C25-C26-C27
3	A	401	NK4	C24-C25-C26-C27
3	B	401	NK4	C25-C26-C27-C28
3	A	401	NK4	O09-C08-O07-C06
3	C	401	NK4	O09-C08-O07-C06
3	D	401	NK4	O09-C08-O07-C06
3	D	401	NK4	C25-C26-C27-C28
3	B	401	NK4	C24-C25-C26-C27
3	C	401	NK4	C25-C26-C27-C28
3	A	401	NK4	C27-C28-C29-C30
3	D	401	NK4	C27-C28-C29-C30
3	D	401	NK4	C34-C35-C36-C37
3	C	401	NK4	C29-C30-C31-C32
3	D	401	NK4	C35-C36-C37-C38
3	B	401	NK4	C22-C23-C24-C25
3	A	401	NK4	C25-C26-C27-C28
3	B	401	NK4	C29-C30-C31-C32
3	B	401	NK4	C27-C28-C29-C30
3	C	401	NK4	C22-C23-C24-C25
3	C	401	NK4	C35-C36-C37-C38
3	A	401	NK4	C35-C36-C37-C38
3	A	401	NK4	C21-C22-C23-C24
3	D	401	NK4	C22-C23-C24-C25
3	A	401	NK4	C29-C30-C31-C32
3	B	401	NK4	C39-C21-C22-C23
3	A	401	NK4	C28-C29-C30-C31
3	C	401	NK4	C27-C28-C29-C30
3	D	401	NK4	C29-C30-C31-C32
3	D	401	NK4	C28-C29-C30-C31

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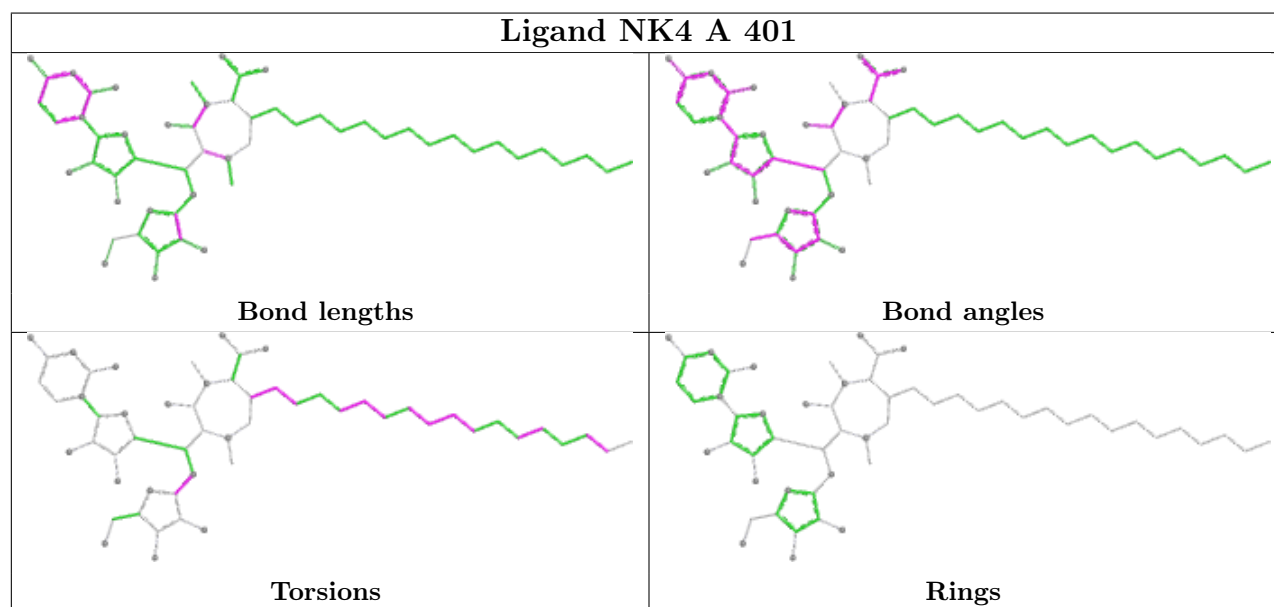
Mol	Chain	Res	Type	Atoms
3	A	401	NK4	C39-C21-C22-C23
3	D	401	NK4	C39-C21-C22-C23

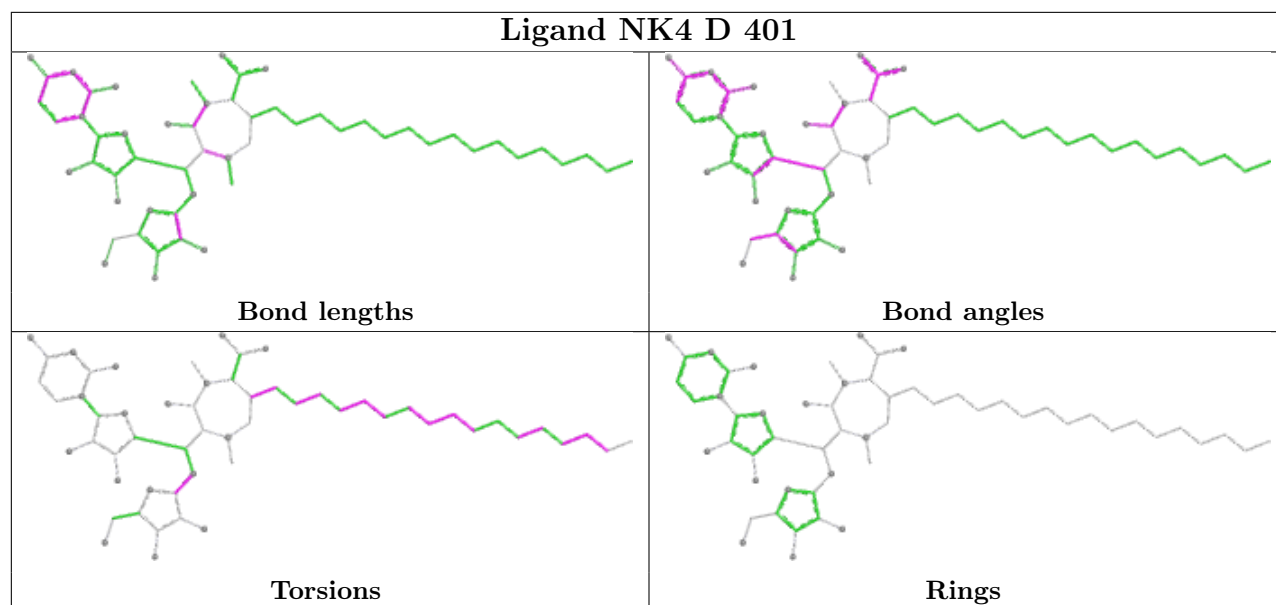
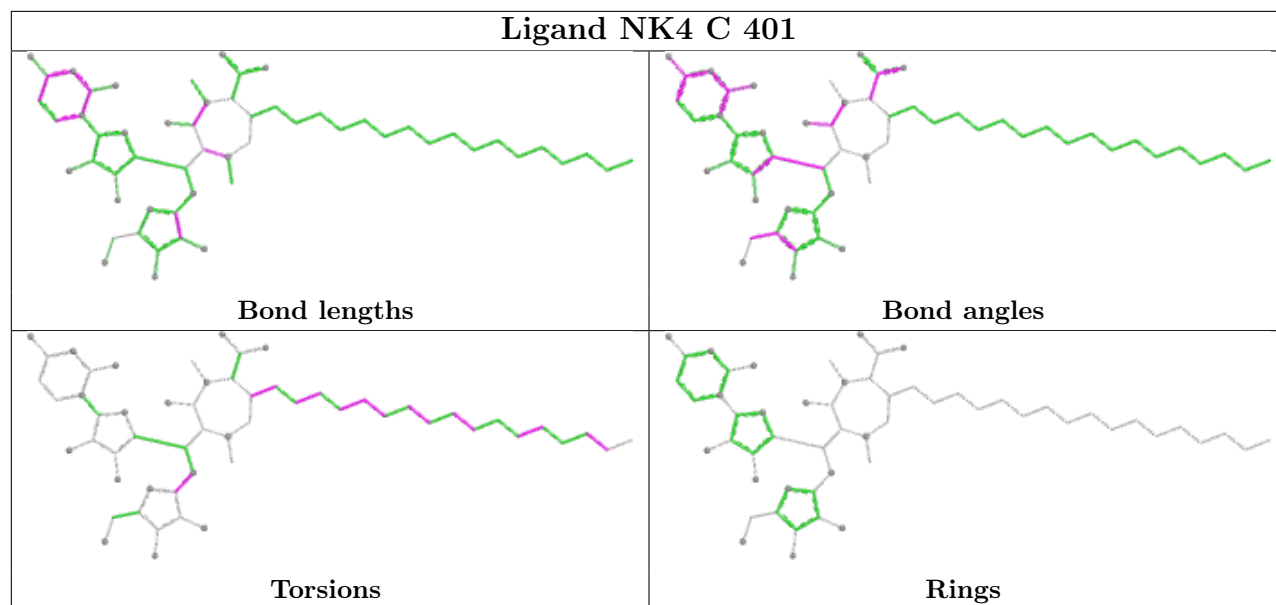
There are no ring outliers.

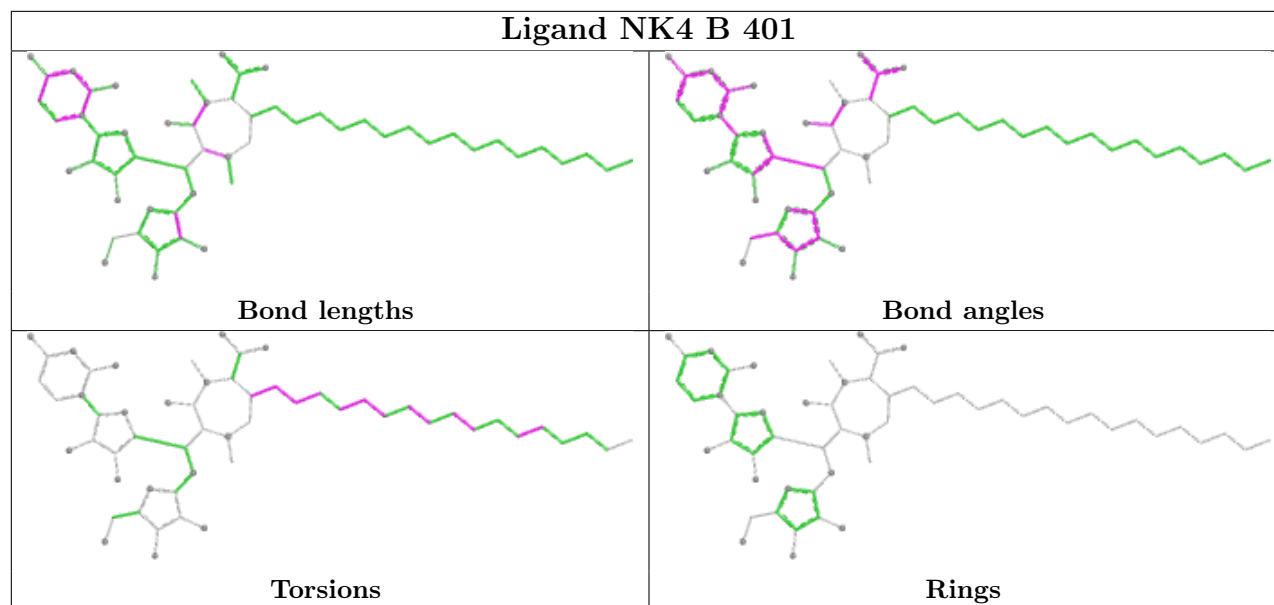
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NK4	1	0
3	C	401	NK4	3	0
3	B	401	NK4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	E	124/137 (90%)	1.15	24 (19%) 3 3	52, 75, 99, 118	0
1	F	125/137 (91%)	1.01	19 (15%) 5 5	55, 75, 111, 143	0
1	G	125/137 (91%)	0.88	16 (12%) 7 7	50, 68, 98, 124	0
1	H	126/137 (91%)	1.14	24 (19%) 3 3	62, 89, 115, 138	0
2	A	326/365 (89%)	0.73	37 (11%) 10 9	52, 74, 120, 151	0
2	B	330/365 (90%)	1.12	55 (16%) 4 4	63, 96, 153, 193	0
2	C	328/365 (89%)	1.12	58 (17%) 4 3	58, 84, 133, 163	0
2	D	337/365 (92%)	1.21	71 (21%) 2 2	64, 93, 145, 188	0
All	All	1821/2008 (90%)	1.05	304 (16%) 4 4	50, 84, 136, 193	0

All (304) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	46	ASN	8.7
2	D	162	PHE	7.7
2	C	346	ILE	7.0
2	D	52	GLN	6.7
2	B	130	ILE	6.3
2	C	23	THR	6.3
2	C	125	LYS	6.2
2	B	96	ASP	6.1
2	B	165	GLU	6.0
2	C	119	TYR	6.0
2	D	163	PHE	5.9
2	D	51	ILE	5.8
2	B	49	ARG	5.8
2	D	161	PRO	5.8
2	B	97	ILE	5.7
2	D	200	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
1	E	25	SER	5.7
2	B	166	LEU	5.7
1	H	112	GLU	5.6
1	E	73	ASN	5.5
2	B	43	SER	5.4
2	D	67	HIS	5.4
1	H	9	GLY	5.3
2	D	164	LYS	5.3
2	C	152	ALA	5.2
2	B	191	LEU	5.2
2	D	233	TYR	5.2
2	A	153	ASP	5.1
1	E	26	GLY	5.1
2	C	155	ASP	5.1
2	D	53	ARG	5.0
2	C	127	GLY	4.9
2	D	59	VAL	4.9
2	D	63	THR	4.9
2	C	112	THR	4.7
1	H	88	GLU	4.7
2	B	232	PRO	4.7
2	D	204	MET	4.7
1	G	13	GLN	4.6
1	H	111	ASN	4.6
2	C	115	PHE	4.6
2	D	174	TYR	4.5
1	H	55	GLY	4.5
2	B	190	ASN	4.5
2	C	312	THR	4.5
2	D	62	TYR	4.5
2	D	358	LEU	4.5
2	C	122	LEU	4.4
1	F	43	LYS	4.3
2	C	134	PHE	4.3
2	B	126	LYS	4.3
2	A	52	GLN	4.3
2	A	166	LEU	4.3
2	C	78	GLY	4.3
2	A	165	GLU	4.3
2	B	321	ALA	4.2
2	D	79	ILE	4.2
2	C	72	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
2	B	313	GLY	4.1
2	B	69	VAL	4.1
2	B	233	TYR	4.1
2	D	22	ILE	4.1
1	G	54	ARG	4.0
1	G	74	ALA	4.0
1	E	56	ASN	4.0
2	D	99	TYR	4.0
2	D	320	ARG	4.0
2	A	151	TRP	4.0
1	G	75	ALA	3.9
2	C	130	ILE	3.9
1	E	70	SER	3.9
2	C	342	TRP	3.8
1	G	101	ALA	3.8
1	H	18	LEU	3.8
2	B	127	GLY	3.8
2	B	13	TRP	3.8
2	D	311	TRP	3.8
2	B	44	PHE	3.8
2	D	169	ASP	3.7
2	B	99	TYR	3.7
2	B	95	TRP	3.7
2	C	17	ASN	3.7
2	C	201	GLY	3.7
2	C	79	ILE	3.7
1	F	73	ASN	3.7
2	C	37	THR	3.7
2	C	274	SER	3.6
1	E	65	GLY	3.6
2	D	203	ALA	3.6
2	C	126	LYS	3.6
2	B	76	MET	3.6
2	A	14	PHE	3.6
1	H	11	LEU	3.5
1	E	83	THR	3.5
2	B	14	PHE	3.5
1	F	55	GLY	3.5
1	F	18	LEU	3.5
1	G	103	THR	3.5
2	D	342	TRP	3.5
2	C	123	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	281	LEU	3.4
1	E	33	ALA	3.4
2	C	358	LEU	3.4
2	A	178	ALA	3.4
2	B	16	PHE	3.4
2	C	82	LEU	3.4
2	D	130	ILE	3.4
2	D	157	ILE	3.4
2	A	17	ASN	3.3
1	H	10	GLY	3.3
2	D	319	LYS	3.3
2	B	52	GLN	3.3
2	D	48	LEU	3.3
2	D	252	LEU	3.3
1	G	102	VAL	3.3
2	A	72	TYR	3.3
2	A	99	TYR	3.3
2	B	85	VAL	3.3
2	D	17	ASN	3.3
2	A	180	PHE	3.3
1	E	68	THR	3.3
1	E	75	ALA	3.3
2	A	152	ALA	3.2
1	H	71	ARG	3.2
2	D	60	ARG	3.2
2	B	311	TRP	3.2
2	D	50	LYS	3.2
2	D	64	PRO	3.2
2	A	233	TYR	3.2
1	E	74	ALA	3.1
1	H	109	GLN	3.1
2	B	174	TYR	3.1
2	C	31	LEU	3.1
2	B	119	TYR	3.1
2	B	77	GLY	3.1
2	C	174	TYR	3.1
2	C	168	VAL	3.0
2	A	19	LEU	3.0
2	D	19	LEU	3.0
1	E	14	THR	3.0
2	C	286	PHE	3.0
2	A	320	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	21	TYR	3.0
2	C	36	LEU	3.0
2	C	204	MET	3.0
1	F	102	VAL	3.0
2	C	150	TYR	2.9
1	H	7	SER	2.9
1	H	102	VAL	2.9
2	A	309	PHE	2.9
2	C	69	VAL	2.9
2	D	160	PHE	2.9
2	B	315	LYS	2.9
2	B	116	TRP	2.9
1	F	79	TYR	2.9
2	D	68	GLU	2.9
2	D	190	ASN	2.9
1	F	40	ALA	2.9
1	H	51	VAL	2.9
2	C	170	LEU	2.9
2	D	332	LEU	2.9
1	G	44	GLU	2.9
2	B	160	PHE	2.9
1	F	57	THR	2.9
2	D	321	ALA	2.8
2	D	269	LEU	2.8
2	B	101	TRP	2.8
2	A	281	LEU	2.8
2	C	51	ILE	2.8
2	B	164	LYS	2.8
1	H	81	GLN	2.8
2	A	179	VAL	2.8
2	C	233	TYR	2.8
2	A	16	PHE	2.8
2	A	311	TRP	2.8
2	D	155	ASP	2.8
2	B	103	VAL	2.7
1	G	125	SER	2.7
2	C	199	ALA	2.7
1	E	72	ASP	2.7
2	A	201	GLY	2.7
1	F	75	ALA	2.7
2	D	150	TYR	2.7
1	E	24	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	72	ASP	2.7
1	E	100	VAL	2.7
2	C	166	LEU	2.7
2	B	50	LYS	2.7
2	A	75	THR	2.7
2	D	312	THR	2.7
2	D	318	PHE	2.6
2	D	193	ASP	2.6
2	A	97	ILE	2.6
2	D	201	GLY	2.6
2	C	128	ILE	2.6
2	D	16	PHE	2.6
1	G	76	ASN	2.6
2	D	227	ASN	2.6
2	B	162	PHE	2.6
1	H	17	SER	2.6
2	D	232	PRO	2.6
2	C	136	LEU	2.6
2	C	339	VAL	2.6
2	C	270	SER	2.5
2	D	350	ILE	2.5
2	A	163	PHE	2.5
2	D	158	LEU	2.5
2	A	177	PHE	2.5
2	B	277	THR	2.5
1	E	101	ALA	2.5
2	D	69	VAL	2.5
2	D	116	TRP	2.5
2	D	302	VAL	2.5
1	E	104	THR	2.5
2	D	83	ILE	2.5
1	E	32	TYR	2.5
1	H	29	PHE	2.5
2	D	72	TYR	2.5
2	D	167	TYR	2.5
2	C	356	LEU	2.4
2	A	134	PHE	2.4
1	H	101	ALA	2.4
2	C	235	GLY	2.4
2	B	305	GLN	2.4
2	B	51	ILE	2.4
2	D	351	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	95	CYS	2.4
2	B	350	ILE	2.4
1	G	27	ARG	2.4
1	F	54	ARG	2.4
2	A	321	ALA	2.4
2	B	216	ALA	2.4
2	C	40	LEU	2.4
2	B	17	ASN	2.3
2	B	316	ARG	2.3
1	H	21	SER	2.3
2	C	158	LEU	2.3
2	A	98	LYS	2.3
2	D	329	LEU	2.3
1	F	103	THR	2.3
2	B	125	LYS	2.3
2	B	39	VAL	2.3
1	G	9	GLY	2.3
2	A	190	ASN	2.3
2	C	124	ASN	2.3
2	A	358	LEU	2.3
1	G	24	THR	2.3
2	B	18	VAL	2.3
1	H	8	GLY	2.3
2	A	279	ALA	2.3
2	C	271	ILE	2.3
2	D	230	TYR	2.3
1	H	73	ASN	2.2
2	D	349	ALA	2.2
2	B	265	ASP	2.2
2	C	284	SER	2.2
2	B	337	ILE	2.2
1	H	72	ASP	2.2
2	C	208	THR	2.2
2	D	30	VAL	2.2
1	E	125	SER	2.2
2	D	15	ALA	2.2
2	C	22	ILE	2.2
2	B	148	ILE	2.2
2	D	74	PRO	2.2
2	D	76	MET	2.2
2	A	327	LEU	2.2
2	B	48	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	157	ILE	2.2
1	E	79	TYR	2.2
2	C	21	TYR	2.2
2	A	105	LEU	2.2
2	C	88	SER	2.2
2	C	243	ALA	2.2
2	C	247	ALA	2.2
1	F	48	VAL	2.1
1	E	69	ILE	2.1
2	A	332	LEU	2.1
1	H	79	TYR	2.1
1	F	125	SER	2.1
1	E	64	LYS	2.1
1	G	100	VAL	2.1
1	H	122	VAL	2.1
1	F	87	PRO	2.1
2	B	317	LEU	2.1
2	A	22	ILE	2.1
2	D	126	LYS	2.1
1	E	15	GLY	2.1
2	B	318	PHE	2.1
2	C	153	ASP	2.1
2	D	23	THR	2.1
2	A	15	ALA	2.1
2	D	207	ALA	2.1
1	F	25	SER	2.0
1	F	28	SER	2.0
1	F	46	GLU	2.0
2	A	308	TYR	2.0
2	C	146	VAL	2.0
2	D	92	LEU	2.0
1	G	8	GLY	2.0
2	D	297	PHE	2.0
1	F	49	ALA	2.0
1	F	97	ALA	2.0
1	H	83	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

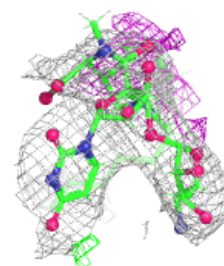
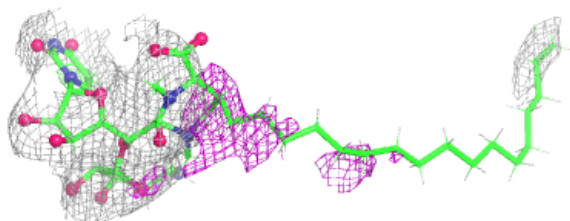
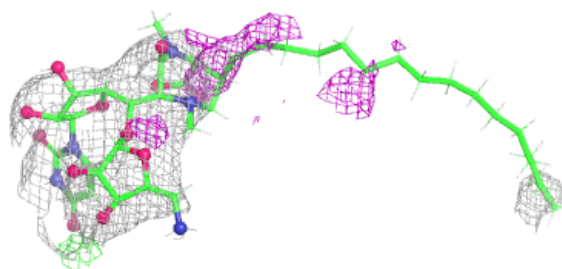
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NK4	B	401	56/56	0.74	0.22	99,133,153,158	0
3	NK4	D	401	56/56	0.85	0.15	83,107,130,133	0
3	NK4	A	401	56/56	0.86	0.15	63,83,111,113	0
3	NK4	C	401	56/56	0.86	0.14	79,104,112,115	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

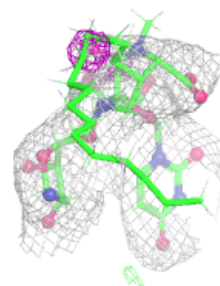
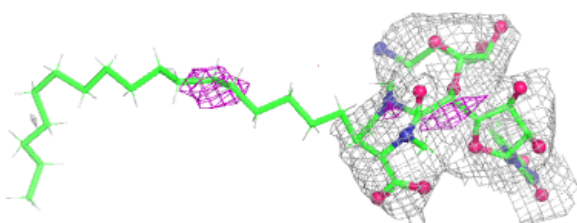
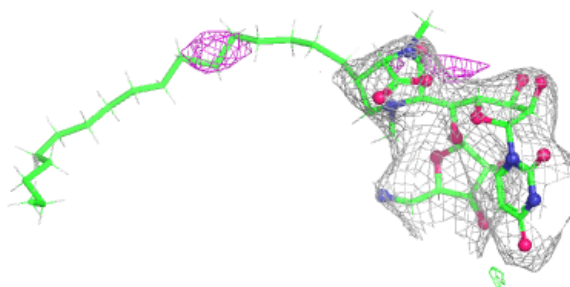
Electron density around NK4 B 401:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

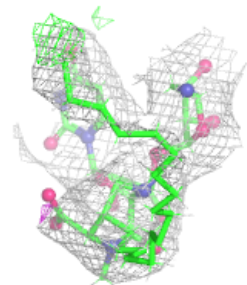
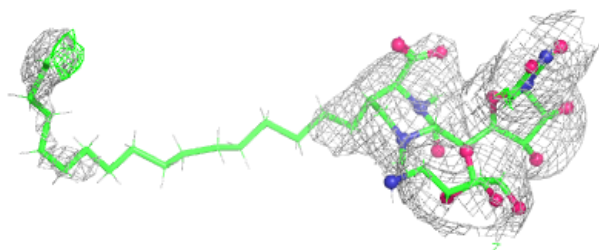
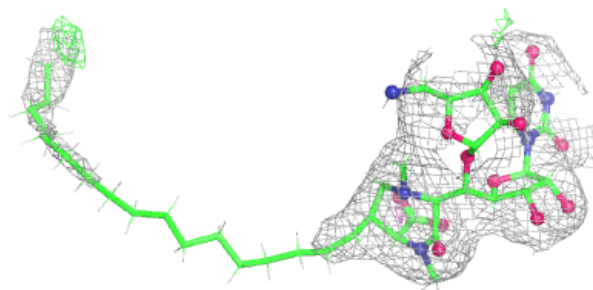


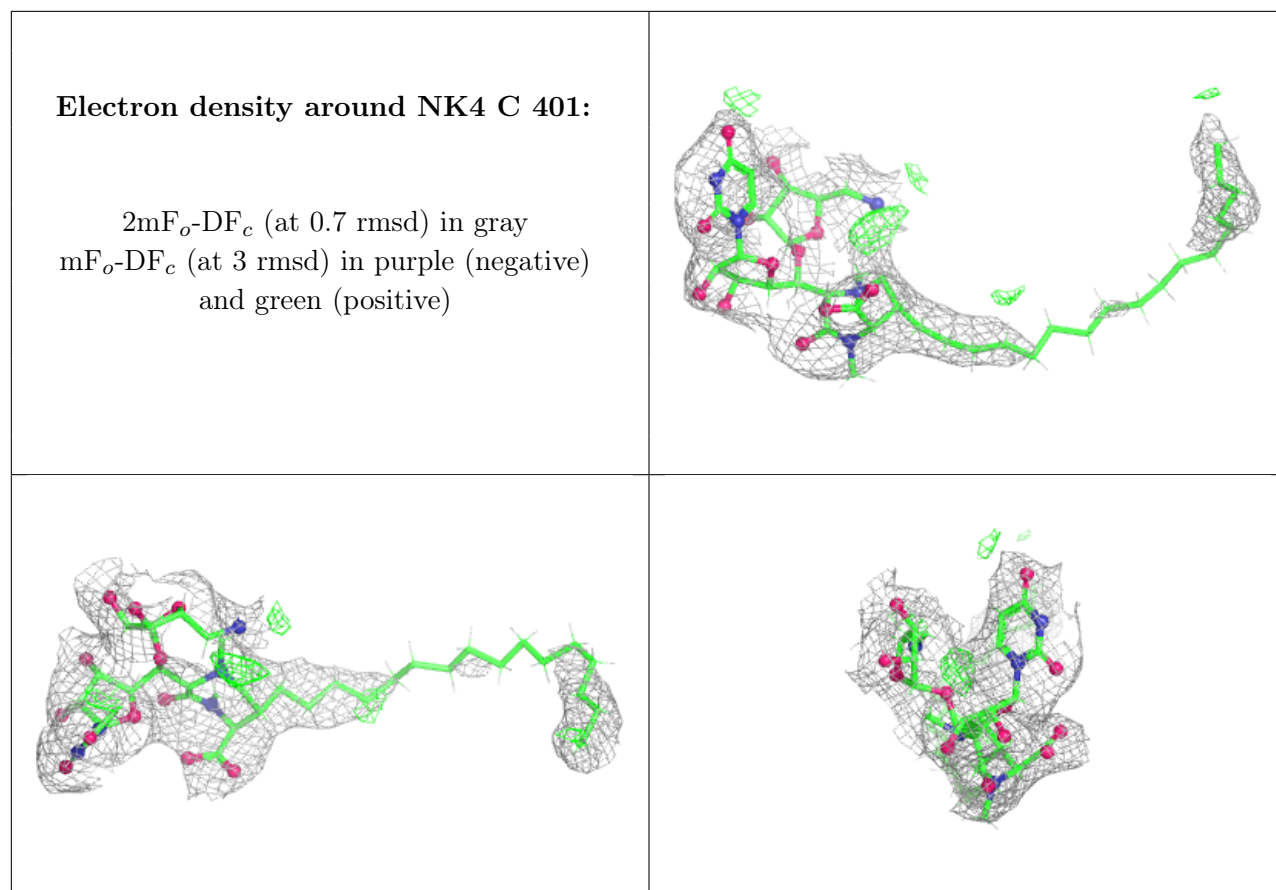
Electron density around NK4 D 401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around NK4 A 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.